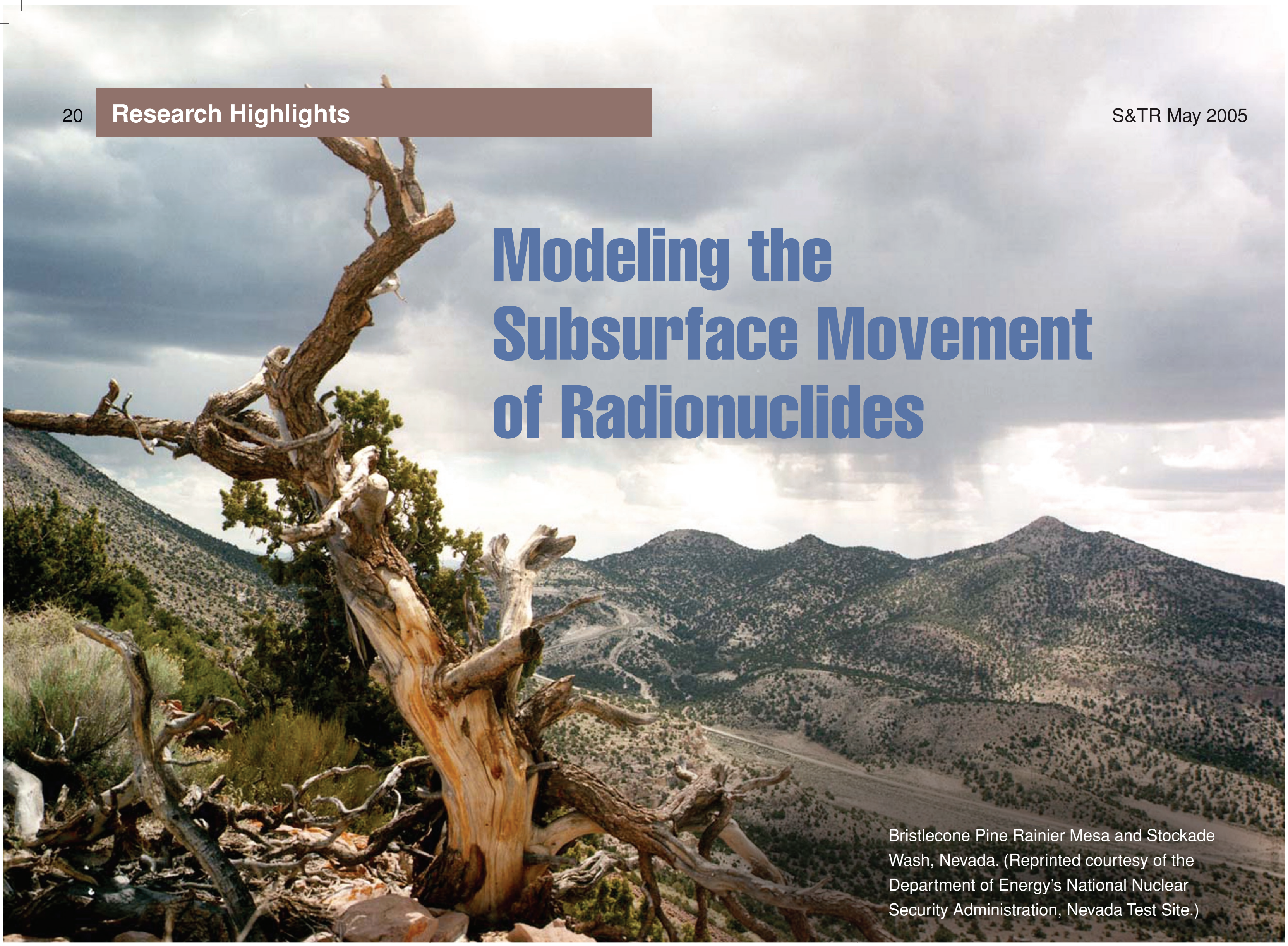
Modeling the Subsurface Movement of Radionuclides



Bristlecone Pine Rainier Mesa and Stockade Wash, Nevada. (Reprinted courtesy of the Department of Energy's National Nuclear Security Administration, Nevada Test Site.)

IN past decades, when underground nuclear tests were routinely conducted at the Nevada Test Site (NTS), scientists and engineers designed their experiments so that data could be recorded without releasing radioactive gases and materials to the atmosphere. Less attention was given to the fate of the radionuclides that remained underground.

But today, scientists know much more about the movement of fluids through geologic media, and they are paying greater attention to the issue of radioactive contamination of the groundwater near these old sites. In 1989, the Department of Energy (DOE), which operates NTS, created a multicontractor effort called the Underground Test Area (UGTA) Project to better understand the risks that past tests may still pose to human health and the environment.

Scientists in Livermore's Energy and Environment (E&E) Directorate are supporting the UGTA Project by modeling in detail how radionuclides from specific underground tests enter the groundwater and migrate through geologic formations. Geologist Gayle Pawloski, who leads the team, says, "Our responsibility is to calculate the 'hydrologic source term.' That is, we determine what radionuclides were released into the groundwater and how they move."

The Livermore models are designed to generate results at a resolution of 2 to 10 meters. These data then become the starting point, or input parameters, for computer models developed to examine large regions of NTS—up to hundreds of square kilometers in area.

A Complex Problem

DOE has established three overall goals for the UGTA Project: identify those areas where radiological contamination from past underground nuclear tests threatens the groundwater, predict the movement of potentially contaminated groundwater, and define the contaminant boundaries or the extent of radionuclide migration.

"It is not economically or technically feasible to clean up the groundwater at NTS," adds Pawloski. "DOE and the Nevada Division of Environmental Protection agreed: the contamination at

NTS is deep and extensive. The project is focused on determining whether groundwater contamination poses a risk to human health or the environment. To that end, the project is developing 1,000-year models of the system, and DOE plans to monitor the site for 100 years or as long as needed."

An underground nuclear explosion is instantaneous, but its effects on a site's geology and hydrology last for centuries. The detonation releases an immense amount of energy—heat and shock waves—vaporizing rock and the nearby groundwater and melting the rock that surrounds the device. Molten rock collects in the cavity formed by the explosion and eventually hardens into a glass puddle on the cavity's floor. The cavity fills with falling rock, which forces the remaining vapor into the surrounding geologic media. The overlying rock continues to collapse, creating a rubble-filled column, or chimney, that may extend to the surface, where a crater forms.

Over time, temperatures cool and gas pressures dissipate, allowing groundwater to filter back into the area. Radionuclides are also moving through the subsurface. They leach out of the glass puddle, react with water and minerals, and continue to decay.

Simulating these complex interactions is not simple, nor is the geology of the NTS test areas—Pahute Mesa, Frenchman Flat, Yucca Flat, Climax Mine, Rainier Mesa, and Shoshone Mountain. The shafts and tunnels from past tests can be hundreds of meters deep through geologic terrain that ranges in complexity from the porous alluvium at Frenchman Flat to the layered and fractured volcanic rocks at Pahute Mesa.

Livermore's E&E Directorate provides the UGTA Project with expertise in containment science, site characterization, and the geology at NTS. Pawloski's team includes Livermore scientists Andrew Tompson, Reed Maxwell, Steve Carle, and Dan Shumaker, who nearly a decade ago developed technologies to model groundwater contamination in complex environments. (See *S&TR*, November 2000, pp. 4–11.) The team also draws on the experience of Laboratory geochemists who worked on DOE's Yucca Mountain Project.

Details Down Under

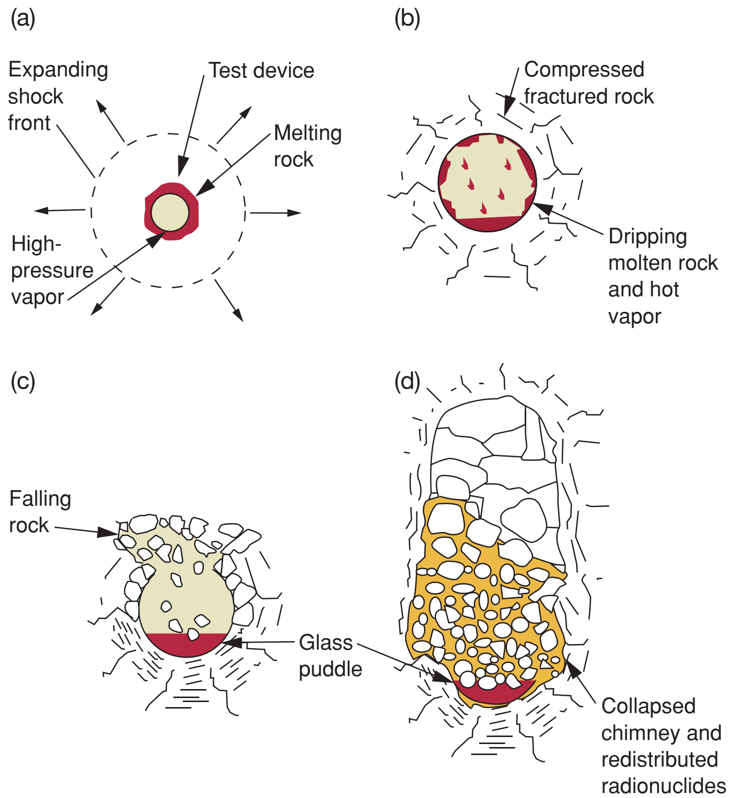
For the UGTA Project, NTS is divided into areas called corrective action units (CAUs). Pawloski's team is modeling each CAU and, to date, has reported on its studies of Frenchman Flat and Pahute Mesa.

To set up the simulations, the team first chooses a representative test from each CAU. For example, at Pahute Mesa, the team focused on the Cheshire test, which was conducted on February 14, 1976. According to unclassified reports, Cheshire's detonation point was 1,167 meters below the surface in fractured volcanic lava, and its announced yield was 200 to 500 kilotons.

The team's overall approach is to first estimate the abundance, spatial distribution, and chemical state of radionuclides immediately following the experiment. To develop those estimates, Livermore geochemist Mavrik Zavarin included an averaged inventory of 43 radionuclides for underground tests at Pahute Mesa. He also used data from past NTS and international nuclear tests to distribute these radionuclides in the melt glass, the cavity, and the altered areas around the cavity.

Going with the Flow

"The legacy data give us a starting point for our calculations—the initial geologic settings and the radiologic source term," says Pawloski. "Our next step is to develop detailed models of groundwater flow and incorporate the most important geochemical processes. Then we use reactive transport models to simulate radionuclide migration away from the test."

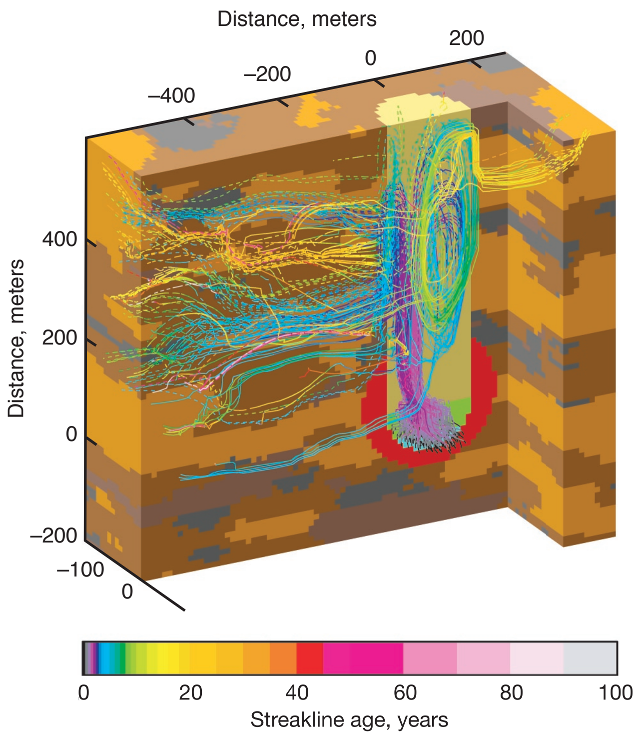


The detonation of an underground nuclear device instantaneously releases an immense amount of energy. (a) In the first microseconds, heat and shock waves from the explosion vaporize rock and groundwater as the cavity grows to its maximum size. (b) Within milliseconds, molten rock begins to harden into a glass puddle on the cavity's floor. (c) The cavity collapses within seconds to hours and fills with falling rock, which displaces the remaining vapor into the surrounding rock. (d) The overlying rock collapses, creating a rubble-filled column, or chimney, that may extend to the surface where a crater eventually forms.

To simulate groundwater flow, the team used Livermore's NUFT code. NUFT is a flexible, three-dimensional (3D) code and can model how geothermal energy and residual test-related heat affect groundwater transport. Temperature data from the Cheshire test were included to improve the model's calibration. Temperatures as high as 150°C had been measured in the melt glass nearly 5 months after the Cheshire test, and small temperature perturbations were observed in the upper part of a downgradient well 11 years later.

The flow model also accounted for the complex geology at Pahute Mesa. Hydraulic tests at the Cheshire site and a nearby water well showed that the permeability of the fractured lava varies as much as four orders of magnitude.

According to the results of the flow model, high temperatures following the Cheshire test may have dramatically increased the rate at which radionuclides were released from the melt glass. "In addition," says Pawloski, "the simulations indicated the presence of a recirculating flow system that drove groundwater upward from the cavity and melt glass through the chimney and into adjacent undisturbed rock."



Livermore's streakline model shows the flow of radionuclides over time as they are released from the melt glass and move away from the cavity of the Cheshire test.

The Cheshire flow model also shows that heat convection through the highly permeable chimney ends about 25 years after the event. After about 100 years, the melt glass cools to background temperature, and groundwater flow returns to pretest conditions.

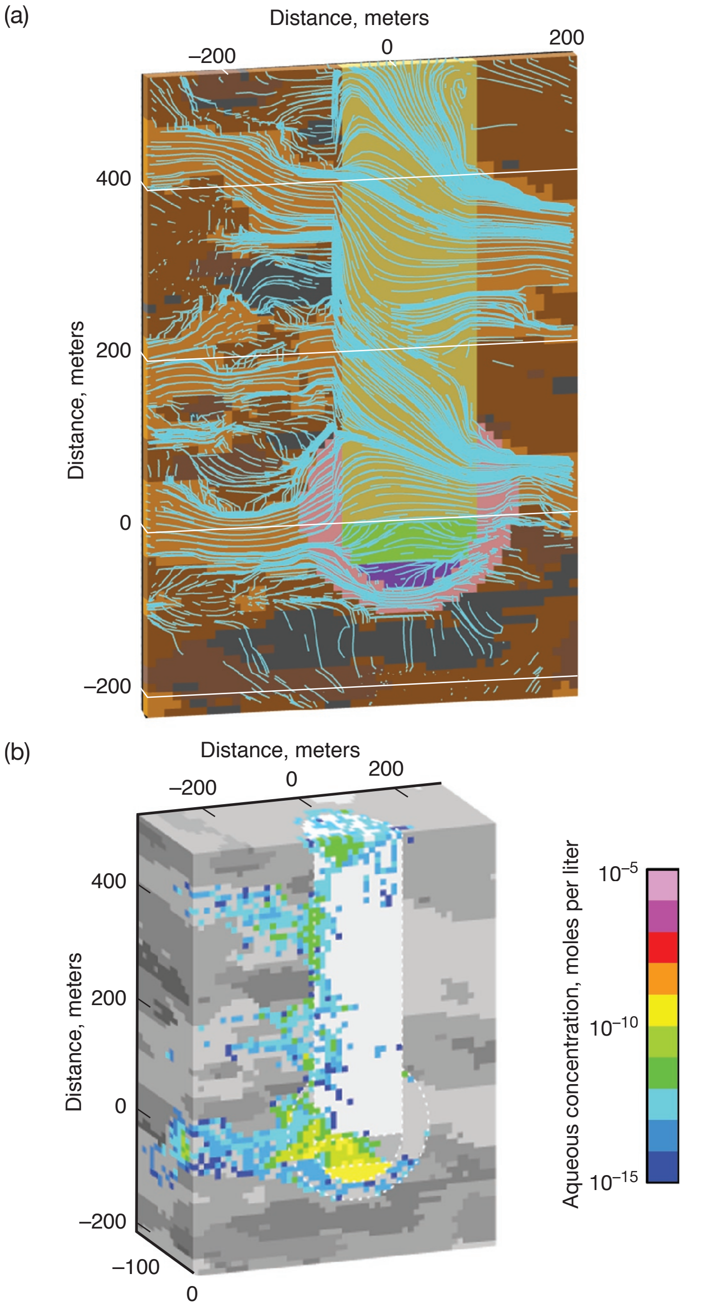
To model reactive transport after the Cheshire test, the team chose two methods: a GIMRT streamline-based model and a SLIM particle model. The GIMRT code performs one-dimensional simulations of transport along thousands of adjacent flow pathways, or streamlines. The SLIM code tracks motion of contaminant particles in the flow field. Both models used the same radionuclide inventories and distributions and were coupled to the NUFT groundwater flow simulations. "None of the codes available today can directly couple 3D hydrothermal flow and 3D reactive transport at the level of detail we require," says Zavarin. "The streamline model helps us understand the changes to the site's geochemistry. The particle model allows us to evaluate the data and process model uncertainties."

The GIMRT model calculated several geochemical reactions, such as aqueous speciation, complexation, ion exchange, mineral dissolution and precipitation, radionuclide decay and ingrowth, and glass dissolution, to determine how radionuclides were released from the melt glass and how they interacted over time with the varied mineralogy along the flow path. This computationally demanding code ran between 4,500 and 6,300 streamlines over five time steps from 100 to 1,000 years. Such calculations would take several years to run on a desktop computer, but with Livermore's clustered supercomputing system, run times were 10 to 100 times faster.

The particle-based model is more efficient than the streamline model, using simplified geochemical processes to simulate a flow scenario for the full 1,000 years. As a result, says Tompson, the team can complete hundreds of particle runs in the time needed to process one streamline model. Results from a single streamline model run compared well with the 100 particle-based runs in the 100- to 1,000-year time frame. These results, called the near-field hydrologic source term, then become the radionuclide source for regional models of Pahute Mesa.

One Piece of a Complicated Puzzle

"We've learned a great deal from modeling tests such as Cheshire," says Pawloski. For example, in the Cheshire simulations, the team found that radionuclides moved up the highly permeable chimney and then migrated away from the test with the flow of the underground water—a process that was verified by field data. The longevity of high temperatures is another useful measure because it indicates the potential for groundwater flow through the cavity. The models also revealed that radionuclides are released from the melt glass slowly over a long time, regardless



(a) This snapshot from a GIMRT simulation of the Cheshire test shows the streamline locations along a 10-meter-wide zone used to calculate radionuclide transport for the 135- to 208-year time step. The differing permeabilities of the surrounding rock appear in the background, where lighter shading indicates higher permeability. (b) A cross section from a particle-based model provides another view of the Cheshire data, showing the concentration of aqueous americium 23.5 years after the event.

of the geologic medium, and short-lived radionuclides decrease to relatively insignificant levels within 400 years of the test.

"NTS has a complex, underground flow system, with different groundwater flow rates and directions, a complicated heterogeneous geologic system, and a variety of radionuclides—all interacting in specific ways," Pawloski says. "Here at Livermore, we're doing our part by defining the hydrologic source term—which is just one piece of this very large jigsaw puzzle that is the UGTA Project. When the puzzle is complete, DOE and the people of Nevada will have a picture that allows them to predict the groundwater movement and help define boundaries for safe water use."

—Ann Parker

Key Words: Cheshire test, environmental restoration, groundwater flow, hydrologic source term, Nevada Test Site, NUFT code, Pahute Mesa, radionuclides, underground nuclear testing, Underground Test Area (UGTA) Project.

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UGTA Web site: www.nv.doe.gov/programs/envmgmt/blackmtn/erundergroundtestarea(ugta).htm